科目名　Course Title	
量子化学1(Quantum Chemistry I)	
学科・専攻　Department/Program	受講年次　Grade
G30 Chemistry	2nd
授業形態　Class style	必修・選択の別　Compulsory or Elective
講義	* See "Remarks"
時間割コード　Registration code	開講期・曜日・時限　Semester,Day & Period
0681210	春学期 月：1
単位数　Credit	科目区分　Course type
2	Basic Specialized Courses

担当教員　Instructor	PHUNG Quan manh(PHUNG Quan manh)
所属研究室　Laboratory	Quantum Chemistry Laboratory
連絡先　Contact	quan.phung@chem.nagoya-u.ac.jp
居室　Room	B225 (Science Building B)

講義の目的とねらい　Course purpose

"What exactly is so special about Quantum Mechanics?" The purpose of this course is to introduce quantum mechanics. It begins with an introduction to elementary quantum mechanics and builds up to convey a thorough theoretical understanding of atomic electronic structure.

履修要件　Prerequisite

Fundamentals of Chemistry I and II, Fundamentals of Physics I and II, Calculus I, Linear Algebra I and II, or permission of the instructor

履修取り下げの方法について　How to Apply for Course Withdrawal

<「履修取り下げ届」提出の要・不要 Necessity/Unnecessity to submit "Course Withdrawal Request Form">
Necessary
<条件等 Conditions>
This course uses the course withdrawal system: Need to submit a Course Withdrawal Request Form by the 6th lecture period when students have no intention of finishing a course.

成績評価　Grading

Midterm exam: 100 points, final exam (comprehensive): 200, homework: 100. TOTAL: 400.
Old scheme: Grade "S": 100-90%, "A": 89-80%, "B": 79-70%, "C": 69-60%, "F": 59-0%.
New scheme: Grade "A+": 100-95%, "A": 94-80%, "B": 79-70%, "C": 69-65%, "C-": 64-60% "F": 59-0%.

不可（F）と欠席（W）の基準　Criteria for "Absent(W)" &"Fail" grades

The “ Absent ” grade (W) is reserved for students that withdraw by the 6th lecture period. After that day, a letter grade will be awarded based on grades earned from all assignments throughout the semester.

関連する科目　Related courses

There are no related courses.

教室　Class room

Check the Course Timetable.

到達目標　Goal

The goal is to lay the foundation of Quantum Theory and see how it helps explain the atomic and molecular structure and chemical bond and reactivity.

授業内容　Content

1 From Classical to Quantum Mechanics (Ch. 1)
2 Wave Packets and the Schrodinger Equation (Ch. 2)
3 The Quantum Mechanical Postulates (Ch. 3)
4 The Particle in the Box 1 (Ch. 4)
6 The Particle in the Box 2 (Ch. 5)
7 Commuting and Non-commuting Operators and the Uncertainty Principle (Ch. 6)
8 MIDTERM EXAM
9 Quantum Mechanical Model for the Vibration and Rotation of Molecules - 1 (Ch. 7)
10 Quantum Mechanical Model for the Vibration and Rotation of Molecules - 2 (Ch. 7)
11 The Vibrational and Rotational Spectroscopy of Diatomic Molecules - 1 (Ch. 8)
12 The Vibrational and Rotational Spectroscopy of Diatomic Molecules - 2 (Ch. 8)
13 The Hydrogen Atom (Ch. 9)
14 Pre-Final Review
15 FINAL EXAM

教科書　Textbook

T. Engel: Quantum Chemistry and Spectroscopy, 3rd Ed. (International edition), Pearson, 2014

参考書　Recommended reading

David W. Ball: Physical Chemistry, 2nd Ed., Cengage Learning, 2015
P. Atkins, J. de Paula, and J. Keeler: Atkins' Physical Chemistry, 11th Ed. Oxford University Press, 2018
D. A. McQuarrie and J. D. Simon "Physical Chemistry A Molecular Approach"

連絡方法　Contact method

quan.phung@chem.nagoya-u.ac.jp

その他　Remarks

*See Course List and Graduation Requirements for your program for your enrollment year.
The course might be (partially) online.

Homework is crucial for mastering new material and developing skills in applying concepts. Weekly homework will be either on paper or electronic. Homework is due at the beginning of class on the due date. A general guideline says an average of 2 to 3 hours of study time per week is necessary for each 1 credit hour.

Exams focus on problem-solving, and exam questions will be similar to the homework problems. Exam grades will be posted in the Gradebook on the Course website before the next class period.